# FITTING FUNCTIONAL EQUATIONS TO EXPERIMENTAL DATA

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## 1. Introduction

Much of mathematical analysis is devoted to the problem of predicting the future behavior of a system, given a descriptive equation and the current state. This is surprising since a basic scientific problem in such fields as physics, engineering, biology and economics is that of determining the structure of a system, given various observations over time [1-6]. In the past, such system identification or inverse problems were solved by trial and error or by simple approximations. Modern computing machines have dramatically altered the picture with their ability to integrate systems of several thousand differential equations given a complete set of initial conditions. Many types of functional equations may be converted into systems of ordinary differential equations. This means that wide classes of direct problems can be solved as initial-value problems.

This also means that a great many inverse problems may be computationally resolved. Let the equations which describe a particular pr cess be a system of differential equations. The unknown structure of the process is reflected in unknown system parameters which appear in the differential equations or in the initial conditions. These parameters are to be estimated on the basis of observations of the process. The identification problem takes the form of a nonlinear boundary-value problem. This can be solved by a variety of methods. One that has been shown to be quite effective is described below.

## 2. Illustrative Example

Consider a system undergoing a process which may be described by the scalar differential equation

$$(1) \qquad \dot{x} = g(x, a),$$

where a is an unknown system parameter, and the initial state

$$(2) \qquad x(0) = c$$

is also unknown. Suppose that at the time $t_i$ the system is observed to be in the state $b_i$, $i = 1, 2, \ldots, N$; $t_{i+1} \geq t_i$. Neither the observations nor the theory of Eq. (1) need be perfect, so in general

$$(3) \qquad x(t_i) \neq b_i, \qquad i = 1, 2, \ldots, N.$$

To fit the theoretical equation (1) to the experimental
data, we wish to determine the constants a and c so that
we minimize S, the sum of the squares of the deviations

$$(4) \qquad S = \sum_{i=1}^{N} [x(t_i) - b_i]^2.$$

Frequently this can be done using a quadratically
convergent successive approximation scheme. Let $x_0(t)$,
$a_0$ and $c_0$ be the current approximations to the optimal
function $x(t)$ and the parameters a and c. The new
approximations are obtained by considering the linearized
equation

$$(5) \qquad \dot{x}_1 = g(x_0, a_0) + (x_1 - x_0)g_x(x_0, a_0)$$

$$+ (a_1 - a_0)g_a(x_0, a_0).$$

The solution of this equation may be written in the form

$$(6) \quad x_1(t) = p(t) + c_1 h(t) + a_1 q(t), \qquad 0 \leq t \leq t_N,$$

where the functions p, h, and q are solutions of the linear
initial-value problems

$$(7) \quad \dot{p} = g_x(x_0, a_0)p + g(x_0, a_0) - x_0\, g_x(x_0, a_0)$$

$$- a_0 g_a(x_0, a_0), \quad p(0) = 0,$$

$$(8) \qquad \dot{h} = g_x(x_0, a_0)h, \qquad h(0) = 1,$$

$$(9) \quad \dot{q} = g_x(x_0, a_0)q + g_a(x_0, a_0), \quad q(0) = 0, \quad t_1 \geq t \geq t_N.$$

The functions p, h and q are readily determined numerically. Then the constants $c_1$ and $a_1$ are determined by minimizing the expression

$$(10) \qquad E = \sum_{i=1}^{N} \left\{ p(t_i) + c_1 h(t_i) + a_1 q(t_i) - b_i \right\}^2,$$

which involves solving the linear algebraic equations

$$(11) \qquad \frac{\partial E}{\partial c_1} = 0, \qquad \frac{\partial E}{\partial a_1} = 0.$$

The process is repeated until a sufficiently small change takes place from one step to the next. In this way, frequently, the differential equation may be fitted to the experimental data [4].

## 3. Other Functional Equations

Systems of ordinary differential equations may be fitted to the data in the manner just described. So may functional equations which can be reduced exactly or approximately to systems of ordinary differential equations. The wave equation, for example,

$$(12) \qquad u_{tt} = c^2(x) u_{xx}$$

can be reduced to ordinary differential equations either by taking Laplace transforms or by using the semi-discretization technique. This leads to the possibility of identifying inhomogeneous media through observation of wave propagation processes [7]. The reduction of differential-difference equations to ordinary differential

equations and the estimation of time lags are discussed
in [5]. Even integral equations may be converted into
initial value problems [8]; this leads to the computational
solution of many inverse problems in multiple scattering
[6].

## 4. Discussion

The least squares criterion of the above example may
be replaced by some other criterion, such as a minimax
condition [9], depending on the statistical nature of
the problem and any a priori estimates that are available.

If the nonlinear Eq. (1) represents a large system
of differential equations with complicated right-hand
sides, the forming of the partial derivatives needed in
the linearized equations could be a formidable task. A
method for the computer evaluation of partial derivatives
of functions given analytically has been described by
Wengert [10] and shown to be useful in orbit determi-
nation [11].

The linearized differential equations may be unstable.
The method of invariant imbedding provides a reformulation
in terms of an initial-value problem for stable differ-
ential equations [12]. Invariant imbedding also obviates
the need to solve linear algebraic equations, another
source of difficulty, by enabling the unknown constants
to be directly determined.

If the data are continuously received, an invariant imbedding method for sequential filtering may be employed [13, 14].

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